

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 105 °C

Global applicability domain: Inside

Local applicability domain index: 5.23e-01

Confidence level: 5.03e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Cifenline</div> <div>Measured: 104</div> <div>Predicted: 105</div>	<div>Image not found</div> <div>Triprolidine</div> <div>Measured: 60.0</div> <div>Predicted: 122</div>
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